

A_α -spectrum of a graph obtained by copies of a rooted graph and applications

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Abstract

Given a connected graph R on r vertices and a rooted graph H , let $R\{H\}$ be the graph obtained from r copies of H and the graph R by identifying the root of the i -th copy of H with the i -th vertex of R . Let $0 \leq \alpha \leq 1$, and let

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$$

where $D(G)$ and $A(G)$ are the diagonal matrix of the vertex degrees of G and the adjacency matrix of G , respectively. A basic result on the A_α -spectrum of $R\{H\}$ is obtained. This result is used to prove that if $H = B_k$ is a generalized Bethe tree on k levels, then the eigenvalues of $A_\alpha(R\{B_k\})$ are the eigenvalues of symmetric tridiagonal matrices of order not exceeding k ; additionally, the multiplicity of each eigenvalue is determined. Finally, applications to a unicyclic graph are given, including an upper bound on the α -spectral radius in terms of the largest vertex degree and the largest height of the trees obtained by removing the edges of the unique cycle in the graph.

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1 Introduction

Let $G = (V(G), E(G))$ be a simple undirected graph on n vertices with vertex set $V(G)$ and edge set $E(G)$. Let $D(G)$ be the diagonal matrix of order n whose (i, i) -entry is the degree of the i -th vertex of G and let $A(G)$ be the adjacency matrix of G . The matrices $L(G) = D(G) - A(G)$ and $Q(G) = D(G) + A(G)$ are the Laplacian and signless Laplacian matrix of G , respectively. The matrices $L(G)$ and $Q(G)$ are both positive semidefinite and $(0, \mathbf{1})$ is an eigenpair of $L(G)$ where $\mathbf{1}$ is the all ones vector. For a connected graph G , the smallest eigenvalue of $Q(G)$ is positive if and only if G is non-bipartite.

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In [7], the family of matrices $A_\alpha(G)$,

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$$

with $\alpha \in [0, 1]$, is introduced together with a number of some basic results and several open problems.

Observe that $A_0(G) = A(G)$ and $A_{1/2}(G) = \frac{1}{2}Q(G)$.

Let R be a connected graph on r vertices. Let v_1, \dots, v_r be the vertices of R . Let $\varepsilon_{i,j} = \varepsilon_{j,i} = 1$ if $v_i \sim v_j$ and let $\varepsilon_{i,j} = \varepsilon_{j,i} = 0$ otherwise.

We recall that a rooted graph is a graph in which one vertex has been distinguished as the root and that the level of a vertex is one more than its distance from the root. In particular, a generalized Bethe tree is a rooted tree in which vertices at the same level have the same degree.

Let H be a rooted graph. Let $R\{H\}$ be the graph obtained from R and r copies of H by identifying the root of the i -copy of H with the vertex v_i of R .

In this paper, we obtain a general result on the A_α -spectrum of $R\{H\}$. We use this result to prove that if $H = B_k$ is a generalized Bethe tree on k levels, then the eigenvalues of $A_\alpha(R\{B_k\})$ are the eigenvalues of symmetric tridiagonal matrices of order not exceeding k ; additionally, the multiplicity of each eigenvalue is determined. Finally, we apply these results to a unicyclic graph, including the derivation of an upper bound on the α -spectral radius in terms of the largest vertex degree and the largest height of the trees obtained by removing the edges of the unique cycle in the graph.

2 A basic result on the A_α -spectrum of copies of a rooted graph

Let E be the matrix of order $n \times n$ with 1 in the (n, n) -entry and zeros elsewhere. For $i = 1, 2, \dots, r$, let $d(v_i)$ be the degree of v_i as a vertex of R and let n be the order of H . Then the total number of vertices in $R\{H\}$ is rn . We label the vertices of $R\{H\}$ as follows: for $i = 1, 2, \dots, r$, using the labels $(i-1)n+1, (i-1)n+2, \dots, in$, we label the vertices of the i -th copy of H from the vertices at the bottom (the set of vertices at the largest distance from the root) to the vertex v_i .

From now on, let $\alpha \in [0, 1]$ and let $\beta = 1 - \alpha$. With the above labeling, we obtain $A_\alpha(R\{H\}) =$

$$\begin{bmatrix} A_\alpha(H) + \alpha d(v_1)E & \beta \varepsilon_{1,2}E & \cdots & \cdots & \beta \varepsilon_{1,r}E \\ \beta \varepsilon_{1,2}E & \ddots & \ddots & & \beta \varepsilon_{2,r}E \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & A_\alpha(H) + \alpha d(v_{r-1})E & \beta \varepsilon_{r-1,r}E \\ \beta \varepsilon_{1,r}E & \beta \varepsilon_{2,r}E & \cdots & \beta \varepsilon_{r-1,r}E & A_\alpha(H) + \alpha d(v_r)E \end{bmatrix}. \quad (1)$$

In this paper, the identity matrix of appropriate order is denoted by I and I_m denotes the identity matrix of order m . Furthermore, we need the following additional notation: $|M|$ and

$\phi_M(\lambda)$ denote the determinant and the characteristic polynomial of M , respectively, and B^T denotes the transpose of B .

The Kronecker product [12] of two matrices $A = (a_{i,j})$ and $B = (b_{i,j})$ of sizes $m \times m$ and $n \times n$, respectively, is the $(mn) \times (mn)$ matrix $A \otimes B = (a_{i,j}B)$. Then, in particular, $I_n \otimes I_m = I_{nm}$. Some basic properties of the Kronecker product are $(A \otimes B)^T = A^T \otimes B^T$ and $(A \otimes B)(C \otimes D) = AC \otimes BD$ for matrices of appropriate sizes. Moreover, if A and B are invertible matrices then $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$.

Let $\text{Spec}(M)$ be the spectrum of a matrix M .

Theorem 1 Let $\rho_1(\alpha), \rho_2(\alpha), \dots, \rho_r(\alpha)$ be the eigenvalues of $A_\alpha(R)$. Then

$$\text{Spec}(A_\alpha(R\{H\})) = \cup_{j=1}^r \text{Spec}(A_\alpha(H) + \rho_j(\alpha)E). \quad (2)$$

Proof From (1)

$$A_\alpha(R\{H\}) = I_r \otimes A_\alpha(H) + A_\alpha(R) \otimes E.$$

Let

$$V = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \dots & \mathbf{v}_{r-1} & \mathbf{v}_r \end{bmatrix}$$

be an orthogonal matrix whose columns $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_r$ are eigenvectors corresponding to the eigenvalues $\rho_1(\alpha), \rho_2(\alpha), \dots, \rho_r(\alpha)$, respectively. Then

$$\begin{aligned} (V \otimes I_n)A_\alpha(R\{H\})(V^T \otimes I_n) &= (V \otimes I_n)(I_r \otimes A_\alpha(H) + A_\alpha(R) \otimes E)(V^T \otimes I_n) \\ &= I_r \otimes A_\alpha(H) + (VA_\alpha(R)V^T) \otimes E. \end{aligned}$$

Moreover,

$$\begin{aligned} (VA_\alpha(R)V^T) \otimes E &= \\ &= \begin{bmatrix} \rho_1(\alpha) & & & & \\ & \rho_2(\alpha) & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & \rho_r(\alpha) \end{bmatrix} \otimes E \\ &= \begin{bmatrix} \rho_1(\alpha)E & & & & \\ & \rho_2(\alpha)E & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & \rho_r(\alpha)E \end{bmatrix}. \end{aligned}$$

Therefore,

$$(V \otimes I_n)A_\alpha(R\{H\})(V^T \otimes I_n) = \begin{bmatrix} A_\alpha(H) + \rho_1(\alpha)E & & & \\ & A_\alpha(H) + \rho_2(\alpha)E & & \\ & & \ddots & \\ & & & \ddots & \\ & & & & A_\alpha(H) + \rho_r(\alpha)E \end{bmatrix}.$$

Since $A_\alpha(R\{H\})$ and $(V \otimes I_n)A_\alpha(R\{H\})(V^T \otimes I_n)$ are similar matrices, (2) follows. \square

3 A_α -spectrum of copies of a generalized Bethe tree

From now on, let B_k be a generalized Bethe tree of k levels. From Theorem 1, we have

Theorem 2 *Let $\rho_1(\alpha), \rho_2(\alpha), \dots, \rho_r(\alpha)$ be the eigenvalues of $A_\alpha(R)$. Then*

$$\text{Spec}(A_\alpha(R\{B_k\})) = \cup_{i=1}^r \text{Spec}(A_\alpha(B_k) + \rho_i(\alpha)E).$$

For $1 \leq j \leq k$, let n_j and d_j be the number and the degree of the vertices of B_k at the level $k - j + 1$, respectively. Thus d_k is the degree of the root, $n_k = 1$, $d_1 = 1$ and n_1 is the number of pendant vertices. For $1 \leq j \leq k - 1$, let $m_j = \frac{n_j}{n_{j+1}}$.

Definition 3 *Let*

$$P_0(\lambda) = 1, P_1(\lambda) = \lambda - \alpha,$$

and

$$P_j(\lambda) = (\lambda - \alpha d_j)P_{j-1}(\lambda) - \beta^2 m_{j-1} P_{j-2}(\lambda)$$

for $j = 2, \dots, k$.

For brevity, sometimes we write f instead $f(\lambda)$. The polynomials in Definition 3 are used in [8], Theorem 5, to factor the characteristic polynomial of $A_\alpha(B_k)$ as given below.

Theorem 4 *The characteristic polynomial of $A_\alpha(B_k)$ satisfies*

$$\phi_{A_\alpha(B_k)}(\lambda) = P_1^{n_1 - n_2} P_2^{n_2 - n_3} \dots P_{k-2}^{n_{k-2} - n_{k-1}} P_{k-1}^{n_{k-1} - 1} P_k. \quad (3)$$

At this point, we introduce the notation \tilde{M} to mean the matrix obtained from M by deleting its last row and its last column.

For $1 \leq i \leq r$, consider the matrices $A_\alpha(B_k) + \rho_i(\alpha)E$ in Theorem 2. Let

$$M_i(\alpha) = A_\alpha(B_k) + \rho_i(\alpha)E.$$

Then

$$\phi_{M_i(\alpha)}(\lambda) = |\lambda I - A_\alpha(B_k) - \rho_i(\alpha)E|.$$

Applying linearity on the last column, we obtain

$$\phi_{M_i(\alpha)}(\lambda) = |\lambda I - A_\alpha(B_k)| - \rho_i(\alpha)|\lambda I - \widetilde{A_\alpha(B_k)}| = \phi_{A_\alpha(B_k)}(\lambda) - \rho_i(\alpha)\phi_{\widetilde{A_\alpha(B_k)}}(\lambda). \quad (4)$$

Theorem 4 gives $\phi_{A_\alpha(B_k)}(\lambda)$ as a product of powers of the polynomials $P_j(\lambda)$ ($1 \leq j \leq k$). We now focus our attention on $\phi_{\widetilde{A_\alpha(B_k)}}(\lambda)$. From the proof of Theorem 5 in [8], we have

$$\phi_{A_\alpha(B_k)}(\lambda) = \phi_{\widetilde{A_\alpha(B_k)}}(\lambda) \frac{P_k}{P_{k-1}}.$$

From this identity and Theorem 4, we obtain

$$\phi_{\widetilde{A_\alpha(B_k)}}(\lambda) = P_1^{n_1-n_2} P_2^{n_2-n_3} \dots P_{k-2}^{n_{k-2}-n_{k-1}} P_{k-1}^{n_{k-1}-n_k}.$$

Replacing in (4) and factoring, we get

Lemma 5 *Let $\rho_1(\alpha), \rho_2(\alpha), \dots, \rho_r(\alpha)$ be the eigenvalues of $A_\alpha(R)$. For $i = 1, \dots, r$, the characteristic polynomial of $M_i(\alpha) = A_\alpha(B_k) + \rho_i(\alpha)E$ satisfies*

$$\phi_{M_i(\alpha)}(\lambda) = P_1^{n_1-n_2} P_2^{n_2-n_3} \dots P_{k-2}^{n_{k-2}-n_{k-1}} P_{k-1}^{n_{k-1}-n_k} (P_k - \rho_i(\alpha)P_{k-1}).$$

Definition 6 *For $j = 1, 2, \dots, k-1$, let T_j be the $j \times j$ leading principal submatrix of the $k \times k$ symmetric tridiagonal matrix*

$$T_k = \begin{bmatrix} \alpha & \beta\sqrt{d_2-1} & 0 & & 0 \\ \beta\sqrt{d_2-1} & \alpha d_2 & \ddots & & \\ & \ddots & \ddots & \beta\sqrt{d_{k-1}-1} & \\ & & \beta\sqrt{d_{k-1}-1} & \alpha d_{k-1} & \beta\sqrt{d_k} \\ 0 & & 0 & \beta\sqrt{d_k} & \alpha d_k \end{bmatrix}. \quad (5)$$

Since $d_s > 1$ for all $s = 2, 3, \dots, j$, each matrix T_j has nonzero codiagonal entries and it is known that its eigenvalues are simple.

The relationship between these matrices and the polynomials $P_j(\lambda)$ is given in [8], Lemma 7:

Lemma 7 *For $j = 1, \dots, k$,*

$$\phi_{T_j}(\lambda) = P_j(\lambda).$$

Definition 8 For $i = 1, \dots, r$, let $Q_i(\lambda)$ be the polynomial

$$Q_i(\lambda) = P_k(\lambda) - \rho_i(\alpha)P_{k-1}(\lambda)$$

and S_i be the $k \times k$ matrix

$$S_i = \begin{bmatrix} \alpha & \beta\sqrt{d_2-1} & 0 & & 0 \\ \beta\sqrt{d_2-1} & \alpha d_2 & \ddots & & \\ & \ddots & \ddots & \beta\sqrt{d_{k-1}-1} & \\ & & \beta\sqrt{d_{k-1}-1} & \alpha d_{k-1} & \beta\sqrt{d_k} \\ 0 & & 0 & \beta\sqrt{d_k} & \alpha d_k + \rho_i(\alpha) \end{bmatrix}.$$

The relationship between the polynomials Q_i and the matrices S_i is given in the following lemma.

Lemma 9 For $i = 1, \dots, r$, $Q_i(\lambda)$ is the characteristic polynomial of the $k \times k$ matrix S_i , that is,

$$\phi_{S_i}(\lambda) = Q_i(\lambda).$$

Proof Applying linearity on the last column, we obtain

$$\phi_{S_i}(\lambda) = |\lambda I - S_i| = |\lambda I - T_k| - \rho_i(\alpha)|\lambda I - T_{k-1}|.$$

Now Lemma 7 implies that

$$\phi_{S_i}(\lambda) = P_k(\lambda) - \rho_i(\alpha)P_{k-1}(\lambda) = Q_i(\lambda).$$

□

We are ready to state the main result of this section.

Theorem 10 Let B_k be a generalized Bethe tree on k levels, and $\alpha \in [0, 1)$. Let $\rho_1(\alpha) \dots \rho_r(\alpha)$ be the eigenvalues of $A_\alpha(R)$ in which $\rho_1(\alpha)$ is the spectral radius. If the matrices T_1, \dots, T_k and S_1, \dots, S_r are as in Definitions 6 and 8, respectively, then

(1)

$$\text{Spec}(A_\alpha(R\{B_k\})) = (\cup_{j=1}^{k-1} \text{Spec}(T_j)) \cup (\cup_{i=1}^r \text{Spec}(S_i)). \quad (6)$$

(2) For $1 \leq j \leq k-1$, the multiplicity of each eigenvalue of T_j as an eigenvalue of $A_\alpha(R\{B_k\})$ is $r(n_j - n_{j+1})$, and for $1 \leq i \leq r$, the eigenvalues of S_i as eigenvalues of $A_\alpha(R\{B_k\})$ are simple. If some eigenvalues obtained in different matrices are equal, their multiplicities are added together.

(3) The largest eigenvalue of S_1 is the spectral radius of $A_\alpha(R\{B_k\})$.

Proof (1) and (2) are consequences of Theorem 2, Lemma 5, Lemma 7 and Lemma 9. The eigenvalues of each T_j interlace the eigenvalues of any S_i . Then the spectral radius of $A_\alpha(R\{B_k\})$ is the largest of the spectral radii of the matrices S_i . We use the fact that the spectral radius of an irreducible nonnegative matrix increases when any of its entries increases, to obtain item (3). \square

A *Bethe tree* $B(d, k)$ is a rooted tree of k levels in which the root has degree d , the vertices at level j ($2 \leq j \leq k-1$) have degree $d+1$ and the vertices at level k have degree equal to 1 (pendant vertices). Clearly, any Bethe tree is a generalized Bethe tree. Theorem 10 immediately implies the following corollary.

Corollary 11 Let $\alpha \in [0, 1)$, and $\beta = 1 - \alpha$. Let $\rho_1(\alpha) \dots \rho_r(\alpha)$ be the eigenvalues of $A_\alpha(R)$ in which $\rho_1(\alpha)$ is the spectral radius. For $1 \leq j \leq k$, let T_j be the leading principal submatrix of order $j \times j$ of the $k \times k$ symmetric tridiagonal matrix

$$T_k = \begin{bmatrix} \alpha & \beta\sqrt{d} & 0 & & 0 \\ \beta\sqrt{d} & \alpha(d+1) & \beta\sqrt{d} & & \\ & \ddots & \ddots & \ddots & \\ & & & \alpha(d+1) & \beta\sqrt{d} \\ 0 & & & \beta\sqrt{d} & \alpha d \end{bmatrix}.$$

For $1 \leq i \leq r$, let

$$S_i = \begin{bmatrix} \alpha & \beta\sqrt{d} & 0 & & 0 \\ \beta\sqrt{d} & \alpha(d+1) & \beta\sqrt{d} & & \\ & \ddots & \ddots & \ddots & \\ & & & \alpha(d+1) & \beta\sqrt{d} \\ 0 & & & \beta\sqrt{d} & \alpha d + \rho_i(\alpha) \end{bmatrix}.$$

Then

(1)

$$\text{Spec}(A_\alpha(R\{B(d, k)\})) = (\cup_{j=1}^{k-1} \text{Spec}(T_j)) \cup (\cup_{i=1}^r \text{Spec}(S_i)).$$

(2) For $1 \leq j \leq k-1$, the multiplicity of each eigenvalue of T_j as an eigenvalue of $A_\alpha(R\{B(d, k)\})$ is $rd^{k-j-1}(d-1)$, and for $1 \leq i \leq r$, the eigenvalues of S_i as eigenvalues of $A_\alpha(R\{B(d, k)\})$ are simple. If some eigenvalues obtained in different matrices are equal, their multiplicities are added together.

(3) The largest eigenvalue of S_1 is the spectral radius of $A_\alpha(R\{B(d, k)\})$.

4 Applications to unicyclic graphs. An upper bound on the A_α -spectral radius

In this section we consider $R = C_r$, the cycle on r vertices. It is known that the eigenvalues of the adjacency matrix of C_r are $2 \cos(\frac{2\pi(i-1)}{r})$, $1 \leq i \leq r$. Since the cycle C_r is a 2-regular graph, it

follows that the eigenvalues of $A_\alpha(C_r)$ are

$$\rho_i(\alpha) = 2\alpha + 2(1 - \alpha) \cos\left(\frac{2\pi(i-1)}{r}\right)$$

for $i = 1, \dots, r$. Hence the spectral radius of $A_\alpha(C_r)$ is $\rho_1(\alpha) = 2$ for any $\alpha \in [0, 1]$.

From Theorem 10, we have

Corollary 12 Let B_k be a generalized Bethe tree of k levels. Let T_1, \dots, T_k be as in Definitions 6. For $i = 1, \dots, r$, let S_i be the $k \times k$ matrix

$$S_i = \begin{bmatrix} \alpha & \beta\sqrt{d_2-1} & 0 & & 0 \\ \beta\sqrt{d_2-1} & \alpha d_2 & \ddots & & \\ & \ddots & \ddots & \beta\sqrt{d_{k-1}-1} & \\ & & \beta\sqrt{d_{k-1}-1} & \alpha d_{k-1} & \beta\sqrt{d_k} \\ 0 & & 0 & \beta\sqrt{d_k} & \alpha d_k + 2\alpha + 2(1 - \alpha) \cos\left(\frac{2\pi(i-1)}{r}\right) \end{bmatrix}.$$

Then

(1)

$$\text{Spec}(A_\alpha(C_r\{B_k\})) = (\cup_{j=1}^{k-1} \text{Spec}(T_j)) \cup (\cup_{i=1}^r \text{Spec}(S_i)). \quad (7)$$

(2) For $1 \leq j \leq k-1$, the multiplicity of each eigenvalue of T_j as an eigenvalue of $A_\alpha(C_r\{B_k\})$ is $r(n_j - n_{j+1})$, and for $1 \leq i \leq r$, the eigenvalues of S_i as eigenvalues of $A_\alpha(C_r\{B_k\})$ are simple. If some eigenvalues obtained in different matrices are equal, their multiplicities are added together.

(3) The largest eigenvalue of

$$S_1 = \begin{bmatrix} \alpha & \beta\sqrt{d_2-1} & 0 & & 0 \\ \beta\sqrt{d_2-1} & \alpha d_2 & \ddots & & \\ & \ddots & \ddots & \beta\sqrt{d_{k-1}-1} & \\ & & \beta\sqrt{d_{k-1}-1} & \alpha d_{k-1} & \beta\sqrt{d_k} \\ 0 & & 0 & \beta\sqrt{d_k} & \alpha d_k + 2 \end{bmatrix}.$$

is the spectral radius of $A_\alpha(C_r\{B_k\})$.

For the case of copies of the Bethe tree $B(d, k)$ attached to C_r , from Corollary 11, we have

Corollary 13 Let $\alpha \in [0, 1)$, and $\beta = 1 - \alpha$. For $1 \leq j \leq k$, let T_j be as Corollary 11. For $1 \leq i \leq r$, let

$$S_i = \begin{bmatrix} \alpha & \beta\sqrt{d} & 0 & & 0 \\ \beta\sqrt{d} & \alpha(d+1) & \beta\sqrt{d} & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha(d+1) & \beta\sqrt{d} & \\ 0 & & 0 & \beta\sqrt{d} & \alpha d + 2\alpha + 2\beta \cos\left(\frac{2\pi(i-1)}{r}\right) \end{bmatrix}.$$

Then

(1) The spectrum of $A_\alpha(C_r\{B(d, k)\})$ is the multiset union

$$\text{Spec}(A_\alpha(C_r\{B(d, k)\})) = (\cup_{j=1}^{k-1} \text{Spec}(T_j)) \cup (\cup_{i=1}^r \text{Spec}(S_i)).$$

(2) For $1 \leq j \leq k-1$, the multiplicity of each eigenvalue of T_j as an eigenvalue of $A_\alpha(C_r\{B(d, k)\})$ is $rd^{k-j-1}(d-1)$, and for $1 \leq i \leq r$, the eigenvalues of S_i as eigenvalues of $A_\alpha(C_r\{B(d, k)\})$ are simple. If some eigenvalues obtained in different matrices are equal, their multiplicities are added together.

(3) The largest eigenvalue of

$$S_i = \begin{bmatrix} \alpha & \beta\sqrt{d} & 0 & & 0 \\ \beta\sqrt{d} & \alpha(d+1) & \beta\sqrt{d} & & \\ & \ddots & \ddots & \ddots & \\ 0 & & 0 & \alpha(d+1) & \beta\sqrt{d} \\ & & & \beta\sqrt{d} & \alpha d + 2 \end{bmatrix}.$$

is the spectral radius of $A_\alpha(C_r\{B(d, k)\})$.

Let $\rho(M)$ be the spectral radius of the matrix M . It is known that if G is a subgraph of H then $\rho(L(G)) \leq \rho(L(H))$, $\rho(Q(G)) \leq \rho(Q(H))$ and $\rho(A(G)) \leq \rho(A(H))$.

In [10] Stevanović proves that for a tree \mathcal{T} with largest vertex degree Δ ,

$$\rho(L(\mathcal{T})) < \Delta + 2\sqrt{\Delta-1}$$

and

$$\rho(A(\mathcal{T})) < 2\sqrt{\Delta-1}.$$

In [5] Hu proves that if G is a unicyclic graph with largest vertex degree Δ then

$$\rho(L(G)) \leq \Delta + 2\sqrt{\Delta-1} \tag{8}$$

with equality if and only if G is the cycle C_n whenever n is even, and

$$\rho(A(G)) \leq 2\sqrt{\Delta-1} \tag{9}$$

with equality if and only if G is the cycle C_n .

From now on, let $G = (V(G), E(G))$ be a unicyclic graph with largest vertex degree Δ .

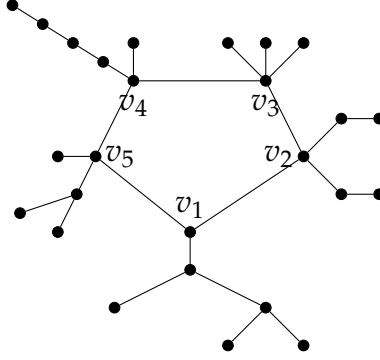
We recall that the height of a rooted tree is the largest distance from its root to a pendant vertex. The following invariant for a unicyclic graph G was introduced in [9].

Definition 14 Let G be a unicyclic graph. Let C_r be the unique cycle in G and let v_1, v_2, \dots, v_r be the vertices of C_r . The graph $G - E(C_r)$ is a forest of r rooted trees T_1, T_2, \dots, T_r with roots v_1, \dots, v_r , respectively. For $i = 1, 2, \dots, r$, let $h(T_i)$ be the height of the tree T_i . Let

$$k(G) = \max \{h(T_i) : 1 \leq i \leq r\} + 1.$$

We say that $k(G)$ is the height of the unicyclic G .

Example 15 Let G be the unicyclic graph:



Then $\Delta(G) = 5$ and the height of G is

$$k(G) = \max\{3, 2, 1, 4, 2\} + 1 = 5,$$

In [9] the upper bounds given in (8) and (9) are improved as follows:

Lemma 16 If G is a unicyclic graph then

$$\rho(L(G)) < \Delta + 2\sqrt{\Delta - 1} \cos \frac{\pi}{2k(G) + 1} \quad (10)$$

for $\Delta \geq 3$ and

$$\rho(A(G)) < 2\sqrt{\Delta - 1} \cos \frac{\pi}{2k(G) + 1} \quad (11)$$

for $\Delta \geq 4$ or $\Delta = 3$ and $k(G) \geq 4$.

It is well known [2] that

$$\rho(L(G)) \leq \rho(Q(G))$$

with equality if and only if G is a bipartite graph. In [3] upper bounds on $\rho(L(G))$ and $\rho(Q(G))$ are given and it is proved that many but not all upper bounds on $\rho(L(G))$ are also bounds for $\rho(Q(G))$. In [1] it is shown that if G is a unicyclic graph, the upper bound on $\rho(L(G))$ in (10) is also an upper bound on $\rho(Q(G))$.

Lemma 17 Let $\Delta \geq 3$. Let

$$X = \begin{bmatrix} 0 & \sqrt{\Delta - 1} & & & \\ \sqrt{\Delta - 1} & 0 & \ddots & & \\ & \ddots & \ddots & \sqrt{\Delta - 1} & \\ & & \sqrt{\Delta - 1} & 0 & \sqrt{\Delta - 2} \\ & & & \sqrt{\Delta - 2} & 2 \end{bmatrix}$$

be a tridiagonal matrix of order $k \times k$. If $\Delta \geq 4$ or $\Delta = 3$ with $k \geq 4$ then

$$\rho(X) < 2\sqrt{\Delta - 1} \cos \frac{\pi}{2k + 1}. \quad (12)$$

Proof Let

$$Y = \begin{bmatrix} 0 & \sqrt{\Delta-1} & & & \\ \sqrt{\Delta-1} & 0 & \ddots & & \\ & \ddots & \ddots & \sqrt{\Delta-1} & \\ & & \sqrt{\Delta-1} & 0 & \sqrt{\Delta-1} \\ & & & \sqrt{\Delta-1} & \sqrt{\Delta-1} \end{bmatrix}$$

be a symmetric tridiagonal matrix of order $k \times k$. It is known [6] that

$$\rho(Y) = 2\sqrt{\Delta-1} \cos \frac{\pi}{2k+1}.$$

Hence proving (12) is equivalent to proving that $\rho(X) < \rho(Y)$. Suppose that $\Delta \geq 5$. Then $X \leq Y$ with strict inequalities in the entries $(k-1, k)$ and $(k, k-1)$. Since the spectral radius of an irreducible nonnegative matrix increases when any of its entries increases, we have $\rho(X) < \rho(Y)$. Thus, (12) has been proved for $\Delta \geq 5$. For $j = 1, 2, \dots, k$, let $x_j(\lambda)$ and $y_j(\lambda)$ be the characteristic polynomials of the $j \times j$ leading principal submatrices of X and Y , respectively. Notice that $x_j(\lambda)$ and $y_j(\lambda)$ are identical polynomials for $j = 1, 2, \dots, k-1$. Using the three-term recursion formula for symmetric tridiagonal matrices, we have

$$x_k(\lambda) = (\lambda - 2)x_{k-1}(\lambda) - (\Delta - 2)x_{k-2}(\lambda) \quad (13)$$

and

$$y_k(\lambda) = (\lambda - \sqrt{\Delta-1})x_{k-1}(\lambda) - (\Delta - 1)x_{k-2}(\lambda). \quad (14)$$

Subtracting (14) from (13), we obtain

$$x_k(\lambda) - y_k(\lambda) = (\sqrt{\Delta-1} - 2)x_{k-1}(\lambda) + x_{k-2}(\lambda). \quad (15)$$

Since X and Y are symmetric tridiagonal matrices with nonzero codiagonal entries, their eigenvalues are simple. Let

$$\alpha_k < \alpha_{k-1} < \dots < \alpha_2 < \rho(X)$$

be the eigenvalues of X . Then

$$x_k(\lambda) = (\lambda - \rho(X)) \prod_{j=2}^k (\lambda - \alpha_j).$$

Let β_1 be the largest zero of the identical polynomials $x_{k-1}(\lambda)$ and $y_{k-1}(\lambda)$. Since the zeros of these polynomials strictly interlace the zeros of the polynomials $x_k(\lambda)$ and $y_k(\lambda)$, we have $\alpha_2 < \beta_1 < \rho(X)$ and $\beta_1 < \rho(Y)$. Therefore $\alpha_2 < \rho(Y)$, $x_{k-1}(\rho(Y)) > 0$ and

$$x_k(\rho(Y)) = (\rho(Y) - \rho(X))c,$$

where

$$c = \prod_{j=2}^k (\rho(Y) - \alpha_j) > 0.$$

Thus in order to conclude that $\rho(X) < \rho(Y)$, we need to show that $x_k(\rho(Y)) > 0$. From (14) and (15),

$$y_k(\rho(Y)) = 0 = (\rho(Y) - \sqrt{\Delta-1})x_{k-1}(\rho(Y)) - (\Delta-1)x_{k-2}(\rho(Y))$$

and

$$x_k(\rho(Y)) = (\sqrt{\Delta-1} - 2)x_{k-1}(\rho(Y)) + x_{k-2}(\rho(Y)).$$

Then

$$x_k(\rho(Y)) = (\sqrt{\Delta-1} - 2 + \frac{\rho(Y) - \sqrt{\Delta-1}}{\Delta-1})x_{k-1}(\rho(Y)). \quad (16)$$

Let $\Delta = 4$. From (16)

$$\begin{aligned} x_k(\rho(Y)) &= (\sqrt{3} - 2 + \frac{2\sqrt{3}\cos\frac{\pi}{2k+1} - \sqrt{3}}{3})x_{k-1}(\rho(Y)) \\ &= (\frac{2\sqrt{3}}{3} - 2 + \frac{2\sqrt{3}}{3}\cos\frac{\pi}{2k+1})x_{k-1}(\rho(Y)) \\ &\geq (\frac{2\sqrt{3}}{3} - 2 + \frac{2\sqrt{3}}{3}\cos\frac{\pi}{5})x_{k-1}(\rho(Y)) > 0.08x_{k-1}(\rho(Y)) > 0. \end{aligned}$$

It remains to prove (12) for $\Delta = 3$ and $k \geq 4$. From (16)

$$\begin{aligned} x_k(\rho(Y)) &= (\sqrt{2} - 2 + \frac{2\sqrt{2}\cos\frac{\pi}{2k+1} - \sqrt{2}}{2})x_{k-1}(\rho(Y)) \\ &= (\frac{\sqrt{2}}{2} - 2 + \sqrt{2}\cos\frac{\pi}{2k+1})x_{k-1}(\rho(Y)) \\ &\geq (\frac{\sqrt{2}}{2} - 2 + \sqrt{2}\cos\frac{\pi}{9})x_{k-1}(\rho(Y)) > 0.03x_{k-1}(\rho(Y)) > 0. \end{aligned}$$

The proof of Lemma 17 is complete. □

At this point, we observe that if G is an induced subgraph of H then $A_\alpha(G) \leq A_\alpha(H)$.

The next theorem gives an upper bound on the spectral radius of $A_\alpha(G)$ in terms of the largest degree and height of the unicyclic graph G .

Theorem 18 *Let G be a unicyclic graph with $\Delta \geq 3$. Let $\alpha \in [0, 1)$. If $\Delta \geq 4$ or $\Delta = 3$ and $k(G) \geq 4$ then*

$$\rho(A_\alpha(G)) < \alpha\Delta + 2(1-\alpha)\sqrt{\Delta-1}\cos\frac{\pi}{2k(G)+1} \quad (17)$$

Proof Let C_r be the unique cycle in G . Let $H = B_{k(G)}$ be a generalized Bethe tree with vertex degrees

$$d_1 = 1, d_2 = \Delta, \dots, d_{k(G)-1} = \Delta, d_{k(G)} = \Delta - 2$$

from the pendant vertices to the root. Then G is an induced subgraph of $C_r\{H\}$. Hence $\rho(A_\alpha(G)) \leq \rho(A_\alpha(C_r\{H\}))$. Let $\beta = 1 - \alpha$. From Corollary 12, the spectral radius of $A_\alpha(C_r\{H\})$ is the spectral radius of the $k(G) \times k(G)$ matrix

$$S_1 = \begin{bmatrix} \alpha & \beta\sqrt{\Delta-1} & & & \\ \beta\sqrt{\Delta-1} & \alpha\Delta & \ddots & & \\ & \ddots & \ddots & \beta\sqrt{\Delta-1} & \\ & & \beta\sqrt{\Delta-1} & \alpha\Delta & \beta\sqrt{\Delta-2} \\ & & & \beta\sqrt{\Delta-2} & \alpha(\Delta-2)+2 \end{bmatrix}$$

$$= \begin{bmatrix} \alpha & \beta\sqrt{\Delta-1} & & & \\ \beta\sqrt{\Delta-1} & \alpha\Delta & \ddots & & \\ & \ddots & \ddots & \beta\sqrt{\Delta-1} & \\ & & \beta\sqrt{\Delta-1} & \alpha\Delta & \beta\sqrt{\Delta-2} \\ & & & \beta\sqrt{\Delta-2} & \alpha\Delta+2\beta \end{bmatrix}.$$

We have

$$S_1 \leq \begin{bmatrix} \alpha\Delta & \beta\sqrt{\Delta-1} & & & \\ \beta\sqrt{\Delta-1} & \alpha\Delta & \ddots & & \\ & \ddots & \ddots & \beta\sqrt{\Delta-1} & \\ & & \beta\sqrt{\Delta-1} & \alpha\Delta & \beta\sqrt{\Delta-2} \\ & & & \beta\sqrt{\Delta-2} & \alpha\Delta+2\beta \end{bmatrix}$$

$$= \alpha \begin{bmatrix} \Delta & & & & \\ & \Delta & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & \Delta \end{bmatrix} + \beta \begin{bmatrix} 0 & \sqrt{\Delta-1} & & & \\ \sqrt{\Delta-1} & \ddots & \ddots & & \\ & \ddots & \ddots & \sqrt{\Delta-1} & \\ & & \sqrt{\Delta-1} & 0 & \sqrt{\Delta-2} \\ & & & \sqrt{\Delta-2} & 2 \end{bmatrix}$$

$$= \alpha \begin{bmatrix} \Delta & & & & \\ & \Delta & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & \Delta \end{bmatrix} + \beta X$$

where X is as in Lemma 17. Then

$$\rho(S_1) \leq \alpha\Delta + \beta\rho(X).$$

If $\Delta \geq 4$ and $\Delta = 3$ with $k(G) \geq 4$, applying Lemma 17, the upper bound (17) follows. \square

Finally we study the cases $\Delta = 3$ and $k(G) \leq 3$. In [9] it is observed that the upper bound (17) does not hold for the adjacency matrix ($\alpha = 0$) when $\Delta = 3$ if $k(G) = 3$ or $k(G) = 2$.

Let $\alpha \neq 0$ and $\Delta = 3$. Let $k(G) = 3$ or $k(G) = 2$. From Corollary 12, the spectral radius of $A_\alpha(C_r\{H\})$ is the spectral radius of the 3×3 matrix

$$M_3 = S_1 = \begin{bmatrix} \alpha & \beta\sqrt{2} & 0 \\ \beta\sqrt{2} & 3\alpha & \beta \\ 0 & \beta & \alpha + 2 \end{bmatrix}.$$

or of the 2×2 matrix

$$M_2 = S_1 = \begin{bmatrix} \alpha & \beta \\ \beta & \alpha + 2 \end{bmatrix}.$$

We have

$$M_3 = \begin{bmatrix} \alpha & \beta\sqrt{2} & 0 \\ \beta\sqrt{2} & 3\alpha & \beta \\ 0 & \beta & \alpha + 2 \end{bmatrix} = \begin{bmatrix} 3\alpha & 0 & 0 \\ 0 & 3\alpha & 0 \\ 0 & 0 & 3\alpha \end{bmatrix} + \begin{bmatrix} -2\alpha & \beta\sqrt{2} & 0 \\ \beta\sqrt{2} & 0 & \beta \\ 0 & \beta & 2\beta \end{bmatrix}.$$

Then

$$\rho(M_3) = 3\alpha + \beta\rho(Z(\gamma))$$

where

$$Z(\gamma) = \begin{bmatrix} \gamma & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

with $\gamma = -2\frac{\alpha}{\beta}$. Similarly

$$M_2 = \begin{bmatrix} \alpha & \beta \\ \beta & \alpha + 2 \end{bmatrix} = \begin{bmatrix} 3\alpha & 0 \\ 0 & 3\alpha \end{bmatrix} + \beta \begin{bmatrix} \delta & 1 \\ 1 & 2 \end{bmatrix}$$

where $\delta = -2\frac{\alpha}{\beta}$. Then

$$\rho(M_2) = 3\alpha + \beta\rho(W(\delta))$$

where

$$W(\delta) = \begin{bmatrix} \delta & 1 \\ 1 & 2 \end{bmatrix}.$$

We recall a simplified version of the Weyl's inequalities for eigenvalues of Hermitian matrices (see, e.g. [4], p. 181).

Lemma 19 Let A and B be Hermitian matrices of order $n \times n$. Let $C = A + B$. Let

$$\alpha_1 \geq \alpha_2 \geq \dots \alpha_n,$$

$$\beta_1 \geq \beta_2 \geq \dots \beta_n$$

and

$$\gamma_1 \geq \gamma_2 \geq \dots \gamma_n$$

be the eigenvalues of A , B and C , respectively. Then, for $j = 1, 2, \dots, n$,

$$\alpha_j + \beta_n \leq \gamma_j \leq \alpha_j + \beta_1. \quad (18)$$

In either of these inequalities equality holds if and only if there exists a nonzero n -vector that is an eigenvector to each of the three eigenvalues involved. The conditions for equality in Weyl's inequalities were first established by So in [11].

We have

$$Z(x) = \begin{bmatrix} x-y & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + Z(y).$$

We claim that $\rho(Z(\gamma))$ is a strictly increasing function of γ . In fact, for $x < y$, Weyl's inequalities imply that

$$\rho(Z(x)) < 0 + \rho(Z(y)) = \rho(Z(y)).$$

A similar argument shows that $\rho(W(\delta))$ is a strictly increasing function of δ . Numerical computations show that $\rho(Z(-0.25)) < 2\sqrt{2} \cos \frac{\pi}{7}$ and $\rho(Z(-0.2)) > 2\sqrt{2} \cos \frac{\pi}{7}$; and, $\rho(W(-1.2)) < 2\sqrt{2} \cos \frac{\pi}{5}$ and $\rho(W(-1.1)) > 2\sqrt{2} \cos \frac{\pi}{5}$. Since $\rho(Z(\gamma))$ and $\rho(W(\delta))$ are continuous functions, there exists $\gamma_0 \in (-0.25, -0.2)$ such that $\rho(Z(\gamma_0)) = 2\sqrt{2} \cos \frac{\pi}{7}$ and there exists $\delta_0 \in (-1.2, -1.1)$ such that $\rho(W(\delta_0)) = 2\sqrt{2} \cos \frac{\pi}{5}$.

Theorem 20 Let G be a unicyclic graph. Let $\Delta = 3$. If $\alpha > \frac{-\gamma_0}{2-\gamma_0}$ whenever $k(G) = 3$ or if $\alpha > \frac{-\delta_0}{2-\delta_0}$ whenever $k(G) = 2$, then the upper bound (17) holds.

Proof Let $k(G) = 3$. There exists γ_0 such that $\rho(Z(\gamma_0)) = 2\sqrt{2} \cos \frac{\pi}{7}$. Moreover, $\rho(Z(\gamma))$ is a strictly increasing function. Hence

$$\rho(Z(\gamma)) < 2\sqrt{2} \cos \frac{\pi}{7}$$

for $\gamma < \gamma_0$. We recall that $\gamma = \frac{-2\alpha}{1-\alpha}$. Imposing the inequality

$$\frac{-2\alpha}{1-\alpha} < \gamma_0$$

we obtain $\alpha > \frac{-\gamma_0}{2-\gamma_0}$. Hence for such values of α , we have

$$\rho(A_\alpha(C_r\{H\})) = \rho(M_3) = 3\alpha + \beta\rho(Z(\gamma)) < 3\alpha + 2(1 - \alpha)\sqrt{2}\cos\frac{\pi}{7}.$$

Then the upper bound (17) holds whenever $k(G) = 3$ and $\Delta = 3$. The proof for the case $k(G) = 2$ is similar. \square

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